A Computational Approach to Studying the Properties of Photosensitizers in Photodynamic Therapy

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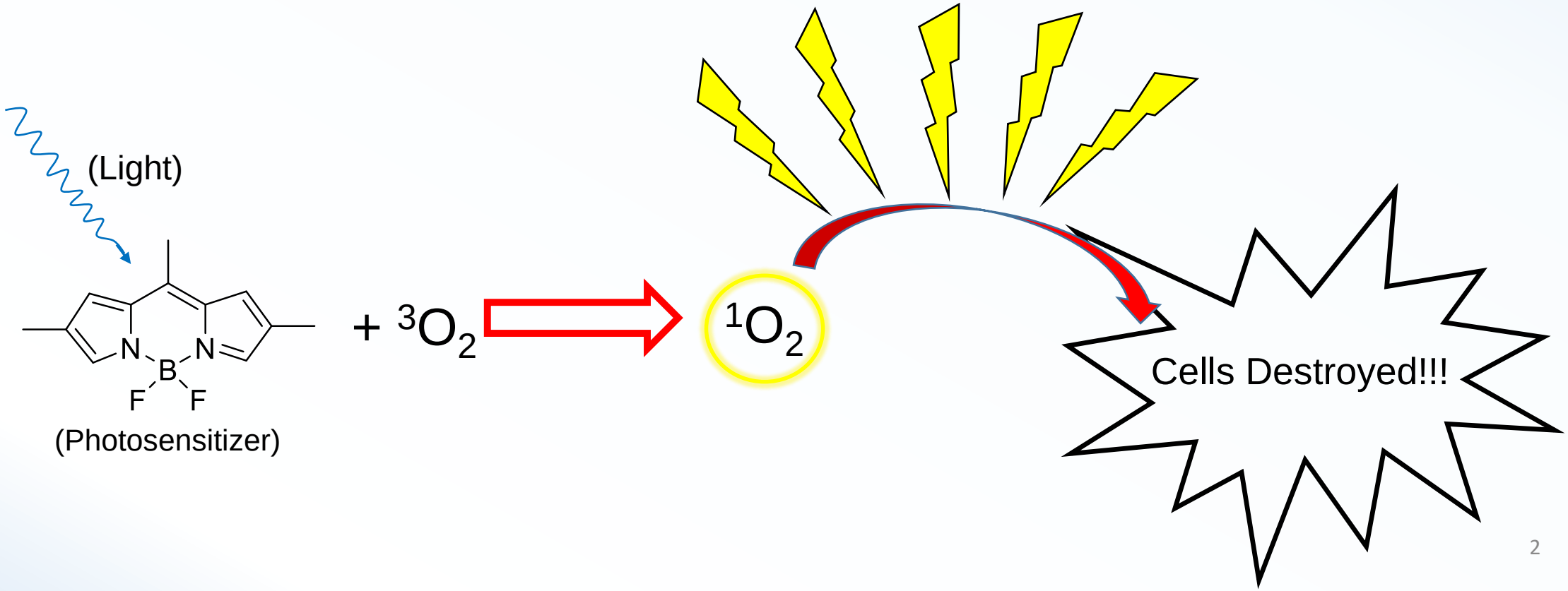
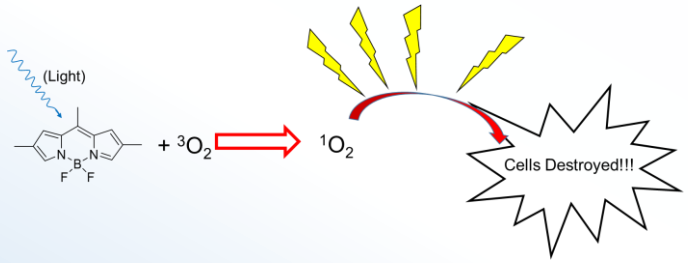
What is photodynamic therapy?

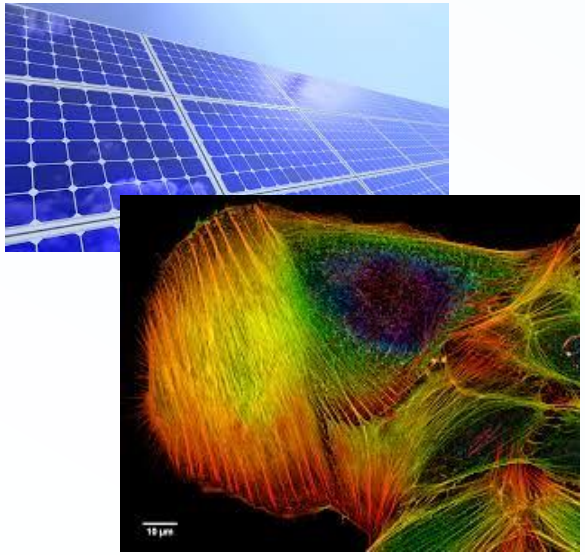
- Photodynamic therapy (PDT): Type of treatment which uses a photosensitizer, light, and oxygen to destroy nearby cancer cells

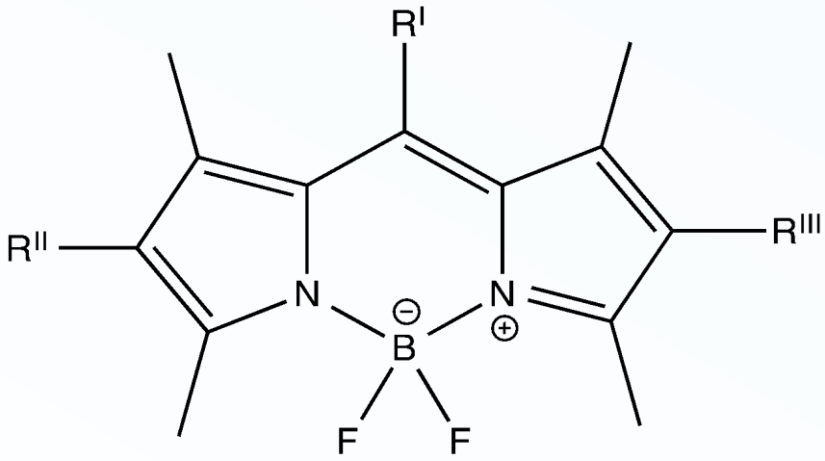


What are photosensitizers?

- Photosensitizer: Molecule which produces a chemical change in other molecules via a photochemical process (i.e. excitation by light)
- We focus on studying boron dipyrromethene (BODIPY) dyes and their specific application to PDT
- BODIPY dyes: Fluorescent compounds used in
  - Biological imaging
  - Solar cells
  - PDT







Studying chemistry via the computer

- Computational Chemistry

  Solving the Schrödinger equation (equation used to calculate energy based on electronic wavefunction)

$$\hat{H}\Psi = E\Psi$$

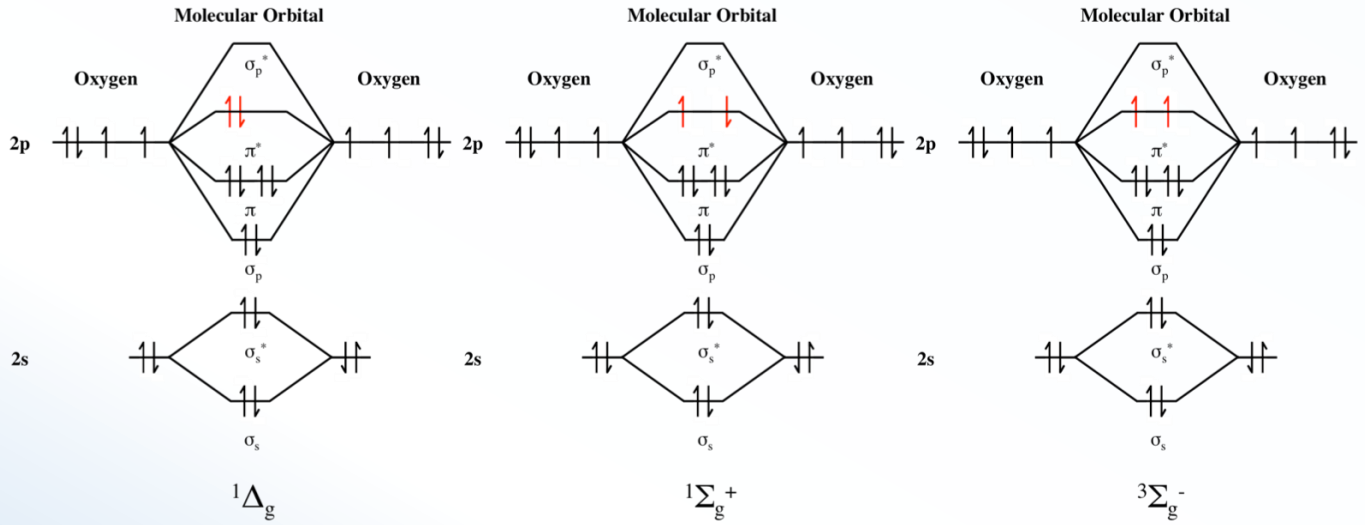
- Computable: $E_{GS,}$ E_{ex}, E_{em}, couplings, vibrational frequencies, charge density, and more
- Accelerates normally extensive processes:
  - Selecting, synthesizing, and testing candidate compounds
  - Measuring properties

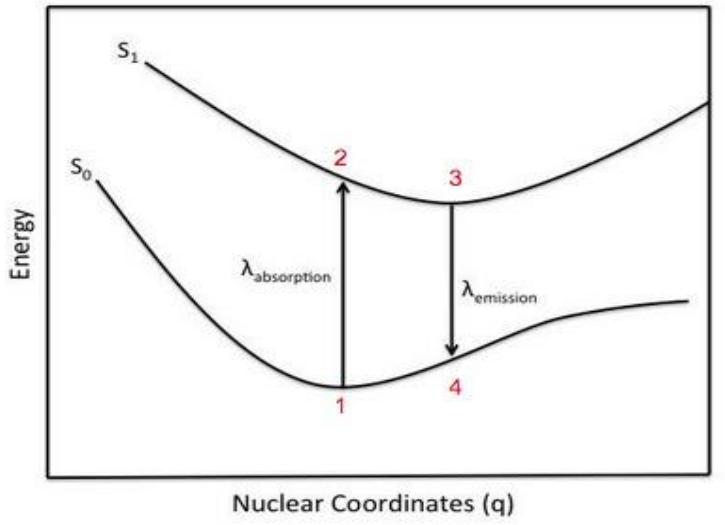
Outline of thesis work

- Compute photophysical properties of a set of BODIPY dyes
- Verify methods in use
- Study the interaction of oxygen with a BODIPY dye
- Investigate the $^{1}O_{2}$ generation properties of a BODIPY dyes

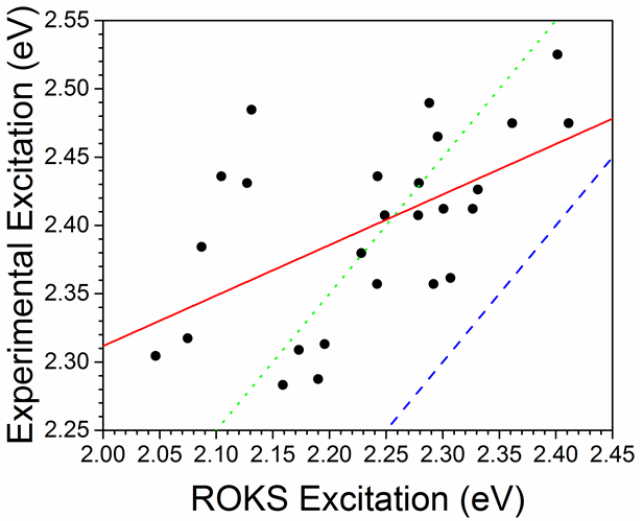
Computational methods

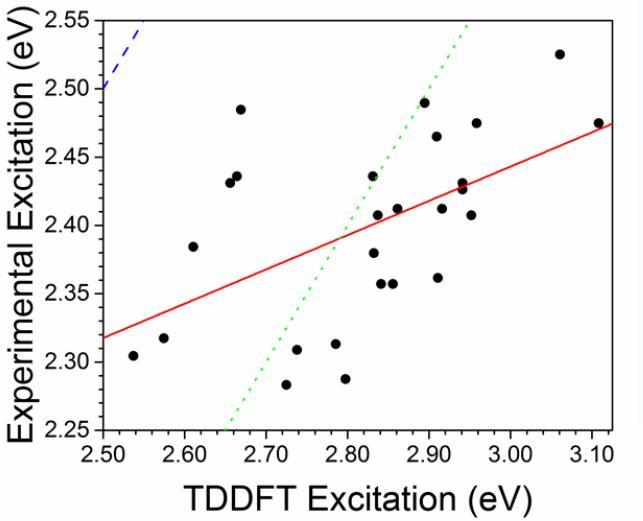
- **Density functional Theory (DFT):** Method to calculate electronic ground states
- **Time-Dependent density functional theory (TD-DFT):** Method to calculate electronic excited states
- **Restricted open-shell Kohn-Sham (ROKS) method:** Method to calculate electronic excited states
- **Constrained density functional theory (CDFT):** Method to constrain atoms/molecules to obtain specific electronic states $^1O_2$, $^3O_2$, etc.

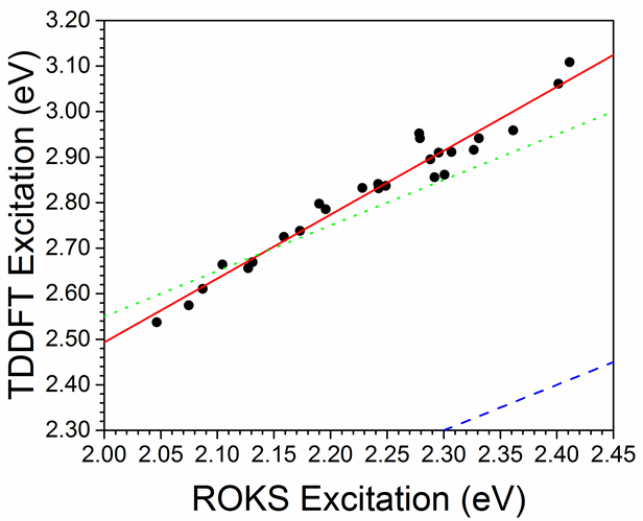


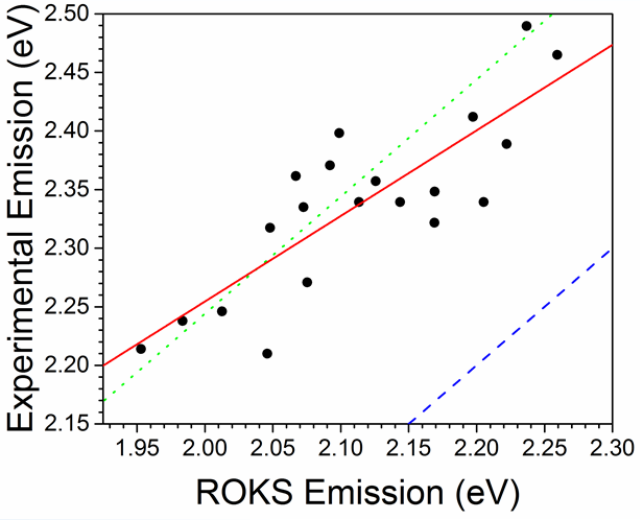


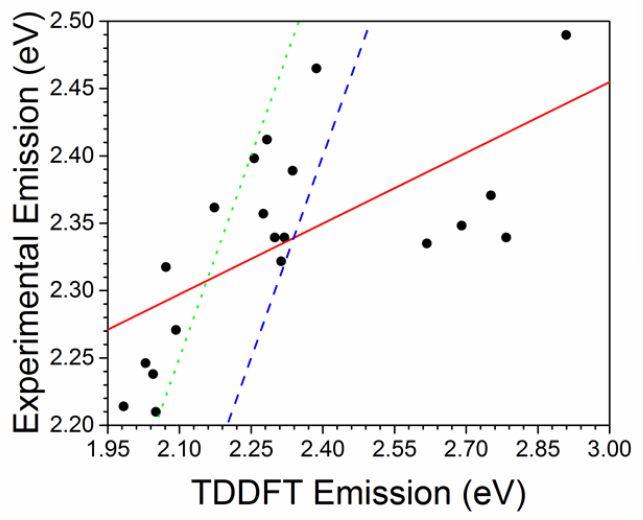
Computing photophysical properties and verifying ROKS

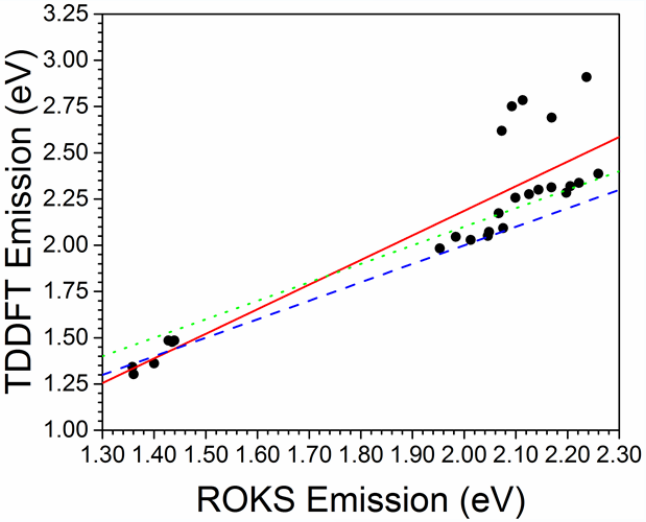




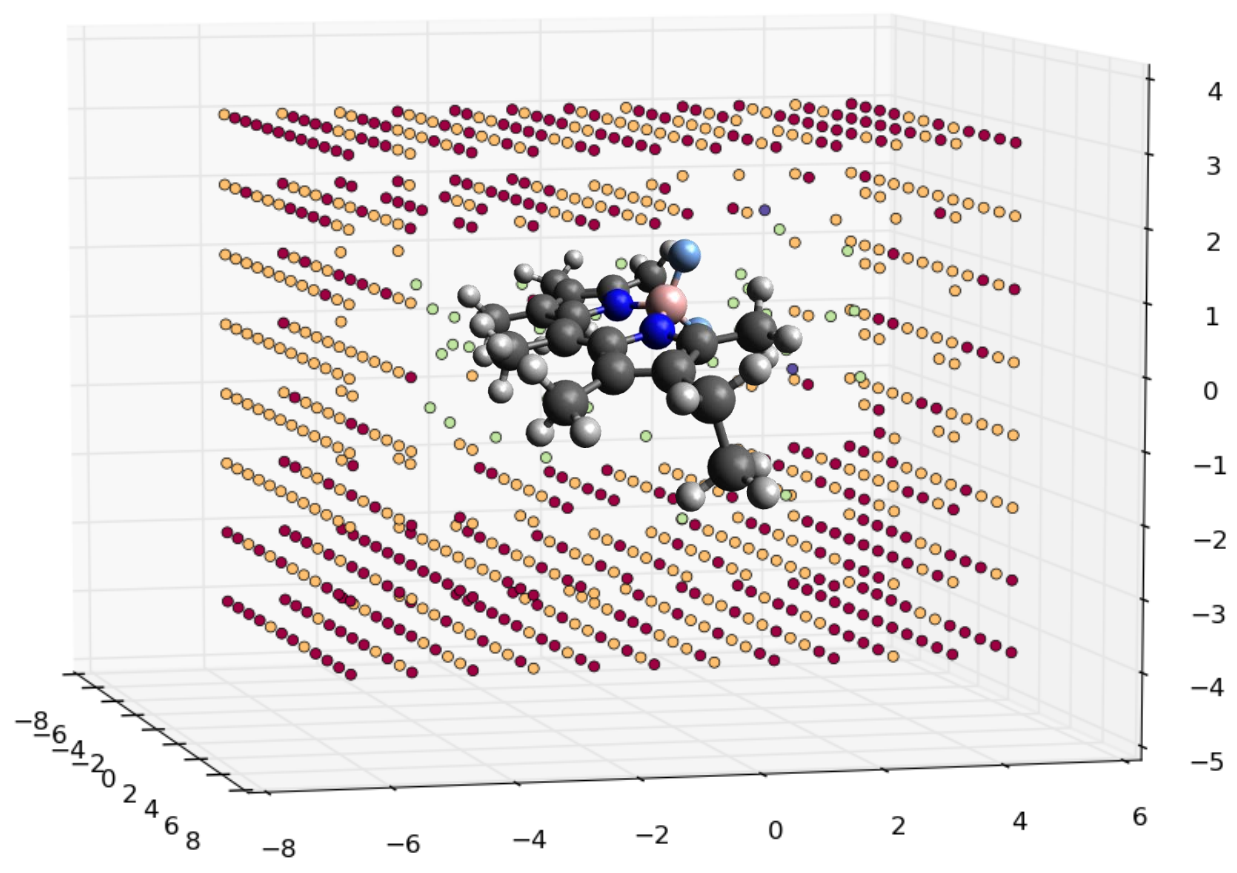


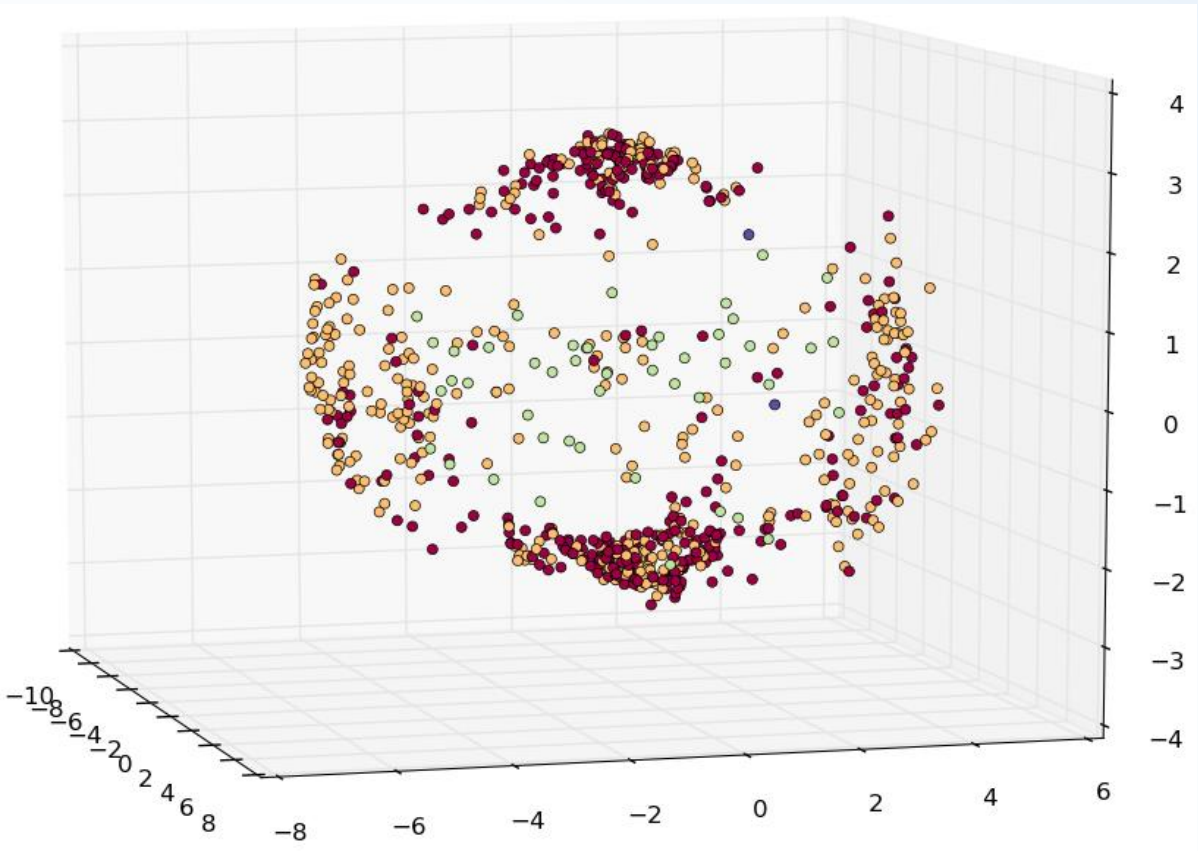






Interaction of O_2 with BODIPY





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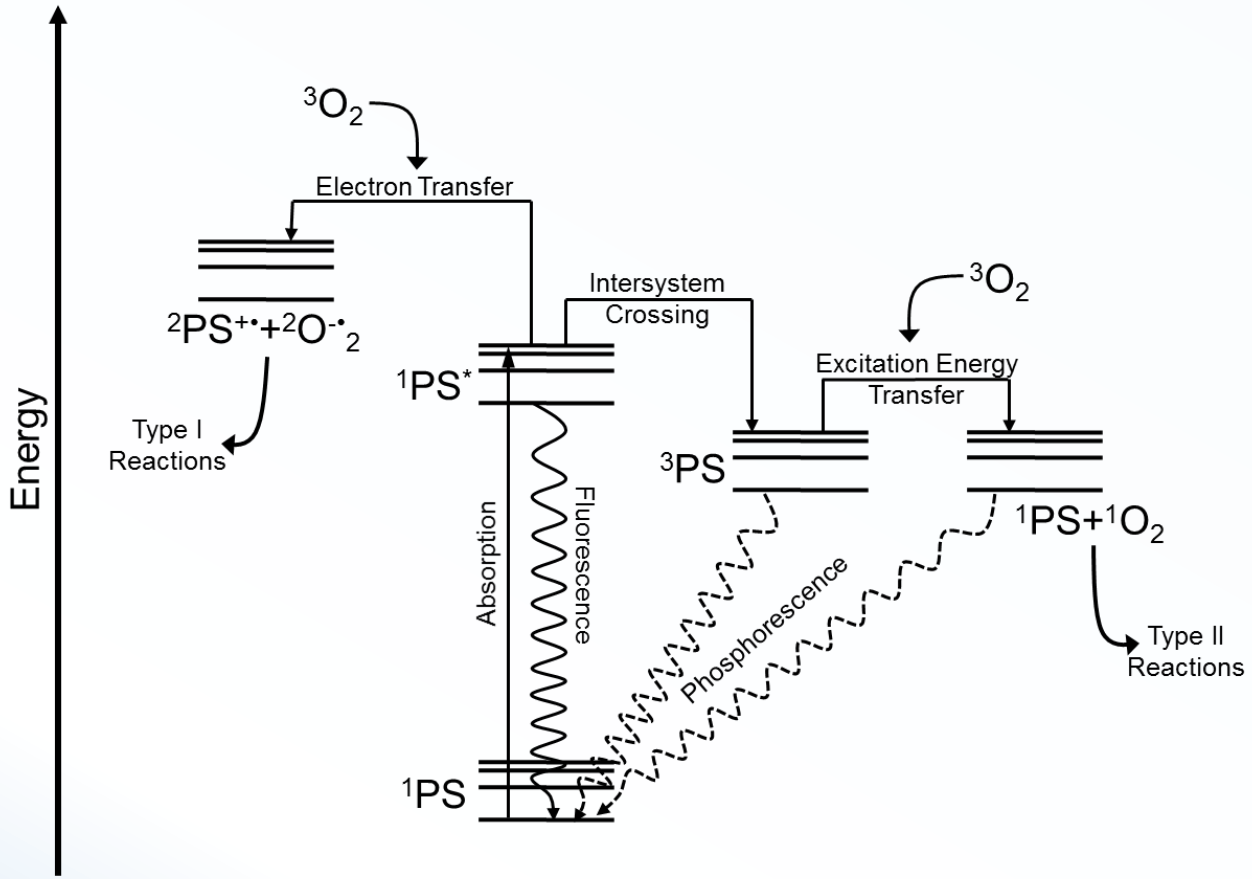
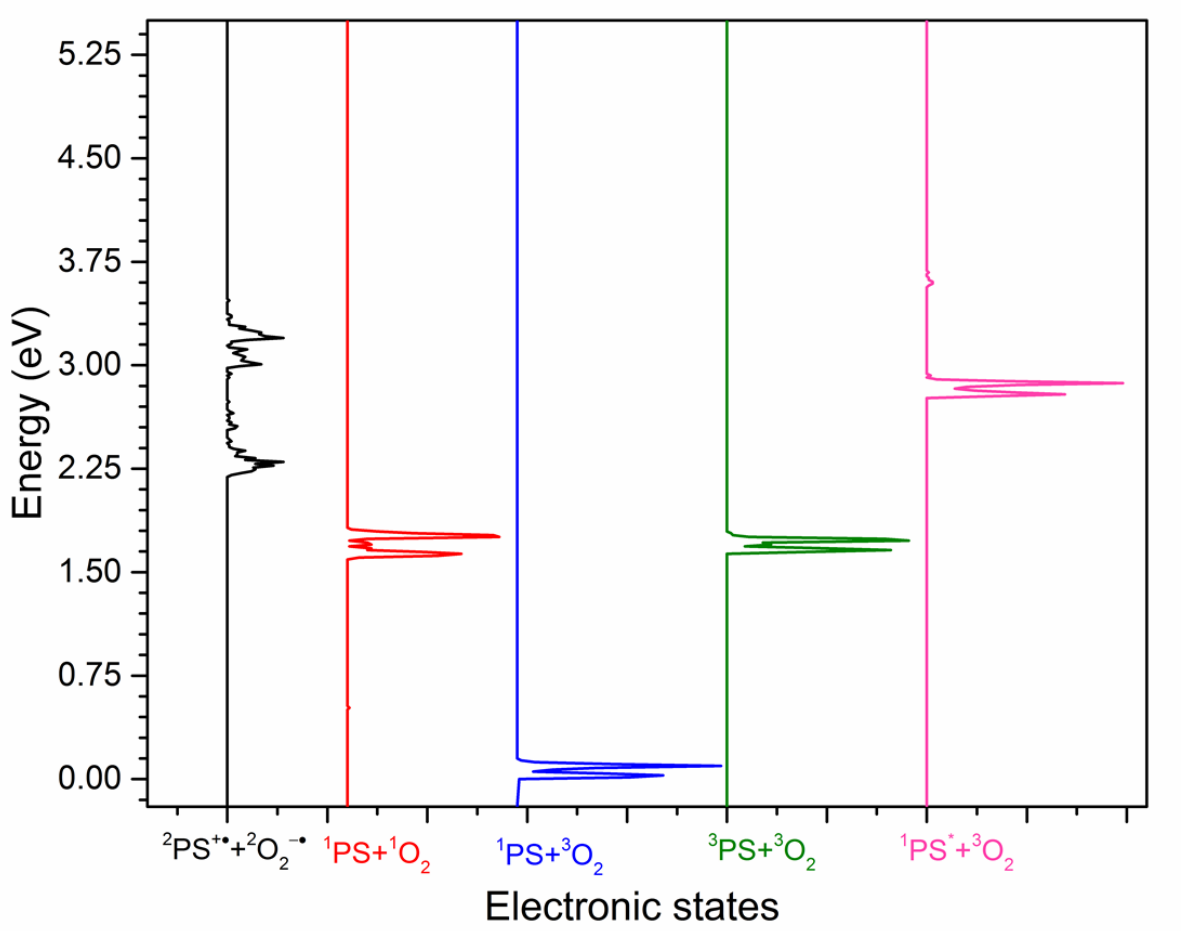
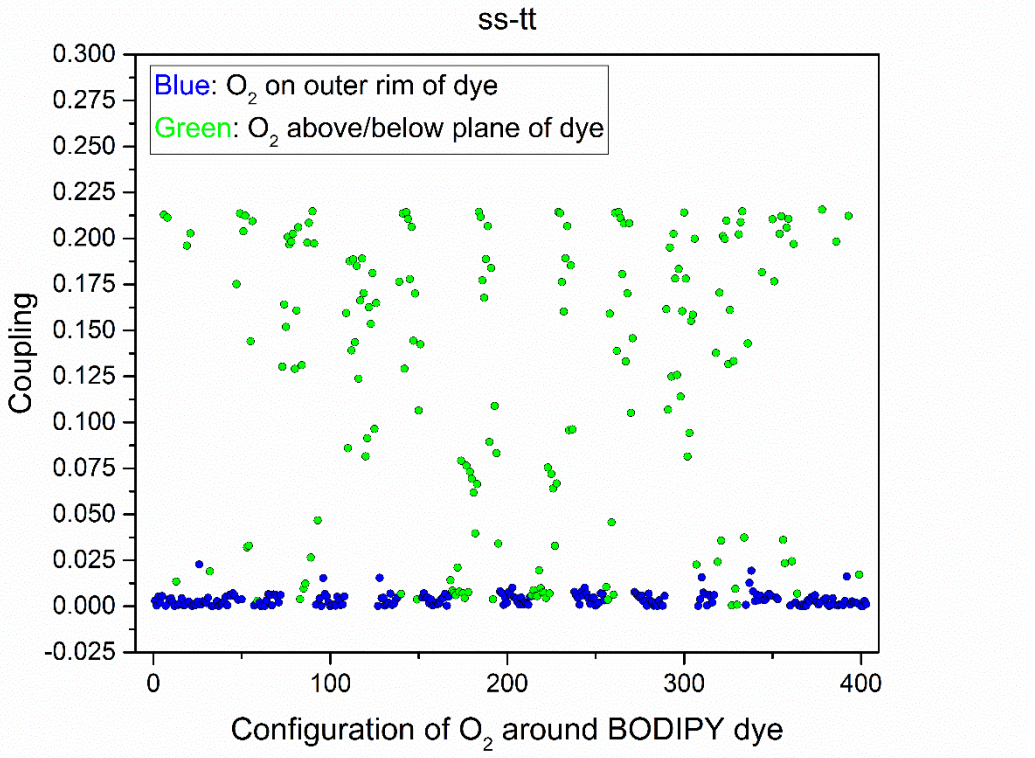
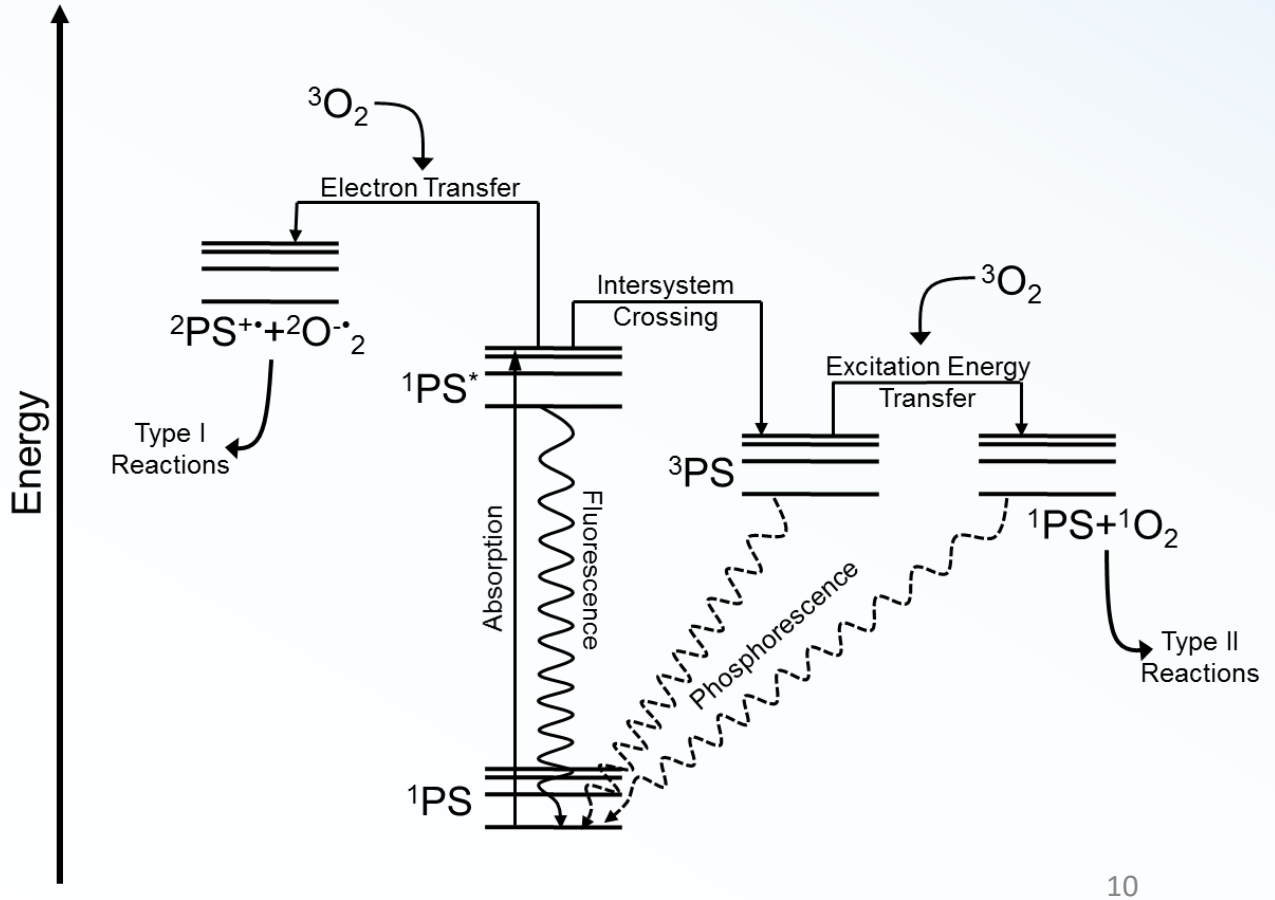




Investigating $^1O_2$ generation

- Compute couplings between electronic states
- Solve for rate of $^1O_2$

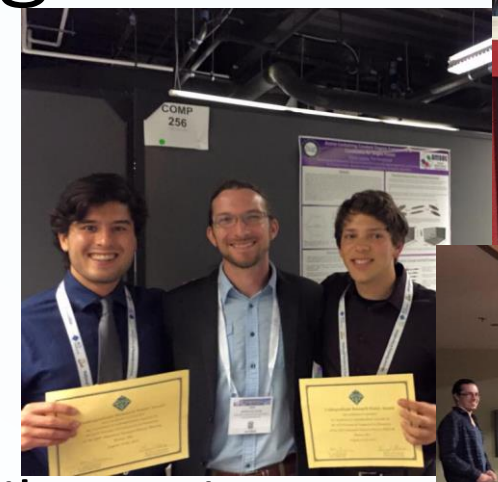




Conclusions, future work and applications

- Verified use of ROKS as a viable excited state method
- Characterizing the $^1O_2$ generation characteristics of a BODIPY chromophore
- Setting foundational work for future scientist working with chromophores used in PDT
- Create a protocol to quickly sort through large sets of candidate dyes to find which have the best properties for use as photosensitizers in PDT

Acknowledgements



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Questions?